UCRL-JRNL-209228

LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

Energy-dependent excitation cross section measurements of the diagnostic lines of Fe XVII

G. V. Brown, P. Beiersdorfer, H. Chen, J. H. Scofield, K. R. Boyce, R. L. Kelley, C. A. Kilbourne, F. S. Porter, S. M. Kahn, A. E. Szymkowiak

January 26, 2005

Physical Review Letters

Disclaimer

Energy-dependent excitation cross section measurements of the diagnostic lines of Fe XVII

G. V. Brown, P. Beiersdorfer, H. Chen, & J. H. Scofield

High Temperature and Astrophysics Division,

Lawrence Livermore National Laboratory,

7000 East Avenue, Livermore, CA 94551

K. R. Boyce, R. L. Kelley, C. A. Kilbourne, & F. S. Porter

NASA/Goddard Space Flight Center, Greenbelt, MD 20771

S. M. Kahn

Department of Physics, Stanford University, Stanford, CA 94305

A. E. Szymkowiak

Department of Physics, Yale University, New Haven, CT 06520

Abstract

By implementing a large-area, gain-stabilized microcalorimeter array on an electron beam ion trap, the electron-impact excitation cross sections for the dominant x-ray lines in the Fe XVII spectrum have been measured as a function of electron energy up to greater than three times the threshold energy, establishing a benchmark for atomic calculations. The results reveal a consistent overestimation by recent calculations of the excitation cross section of the resonance transition, which is shown to be at the root of several long-standing problems associated with modeling solar and astrophysical Fe XVII spectra. The data do not show strong contributions from resonance excitation contrary to recent statements in the literature.

PACS numbers: 34.80.Kw, 32.80.Cy, 95.55.Ka

The emission from neonlike Fe^{16+} dominates the spectra of a plethora of non-terrestrial sources in the soft x-ray region between about 10 and 20 Å. The high-resolution grating instruments on the *Chandra* and *XMM-Newton* X-Ray observatories were specifically designed to focus on this spectral region resulting in the highest quality spectra ever produced [1]. However, the diagnostic utility of the Fe XVII spectrum has been limited because modeling efforts have not been able to explain the intensity pattern of the emission from objects such as stellar coronae or galactic centers [2, 3]. Problems had already existed in analyses of solar spectra [4], where it was found that spectra could only be adequately fitted by invoking resonance scattering. This process mainly affects the $1s^2 2s^2 2p^5_{1/2} 3d_{3/2}\ {}^1P_1 \rightarrow 1s^2 2s^2 2p^6\ {}^1S_0$ resonance transition commonly labeled 3C, which dominates the spectral emission [5]. Resonance scattering was, however, not a good explanation for many astrophysical sources [6]. Moreover, it cannot explain many laboratory measurements of relative line ratios using electron beam ion traps and tokamaks [7–10], which are generally in good agreement with those measured from astrophysical sources and the Sun, and all operate in the optically thin limit.

A resolution of the problems associated with interpreting the Fe XVII spectra was suggested by Chen & Pradhan [11]. They performed a large-scale relativistic close-coupling calculation, which found a large contribution by resonances to the excitation of the Fe XVII lines, especially to the $1s^2 2s^2 2p^5_{1/2} 3d_{3/2}\ {}^3P_1 \rightarrow 1s^2 2s^2 2p^6\ {}^1S_0$ intercombination line at 15.26 Å known as 3D. Their calculations were the first to provide excellent agreement with laboratory data from electron beam ion traps, finding a ratio of 2.95–3.27 for the intensity of 3C to that of 3D, compared to experimental ratios of 2.77–3.15 in the energy range of 0.85 to 1.15 keV.

So far laboratory data only exist for relative line ratios and thus provide only relative values of the excitation cross sections of the Fe XVII lines. Although the electron beam ion trap was specifically designed for electron excitation cross section measurements [12], such measurements have been limited to a few ions where uncertainty inherent in the unknown overlap between ions and the electron beam can be avoided by measuring the signal due to the radiative capture of the beam electrons by the ions in the trap [13]. Radiative capture by Fe^{16+} proceeds into the $3s$, $3p$, and $3d$ levels of Na-like Fe. Observation of this signal is difficult because of its inherent weakness. The capture cross section is about three orders of magnitude smaller than the Fe XVII excitation cross sections, precluding measurements with crystal spectrometers. Standard solid-state type x-ray detectors used in previous measurements do not have the energy resolution to resolve such weak features among the emission from either neighboring charge states or the emission from indigenous light or heavy impurity ions, such as carbon, argon, barium, or tungsten.

For the present measurements, we used a large-area, gain-stabilized, photometrically calibrated x-ray microcalorimeter [14] to measure both the Fe XVII line emission and the radiative electron capture signal. Our measurements give accurate values of the excitation cross sections of the Fe XVII resonance line $3C$ and of the intercombination line $3D$ that represent the first benchmarks for discerning the accuracy of different approaches in atomic theory and for determining the root cause of long-standing discrepencies between models and astrophysical observations.

Our measurements were carried out at the University of California Lawrence Livermore National Laboratory EBIT-I electron beam ion trap. Iron was continuously injected into the trap as iron pentacarbonyl using a ballistic gas injector and ionized by the electron beam. The trap was emptied and refilled once every 3.5 seconds. This minimized the concentration of heavy impurities emanating from the electron gun to below one part in 10^4.

The x-ray spectrometer microcalorimeter (XRS), developed at the NASA-Goddard Space Flight Center, consists of a 6×6 array of 625×625 μm^2 pixels cooled to 60 mK, of which 30 were active during the present measurements [14, 15]. Each pixel has a long-time gain stability that extends beyond magnet cycles, so no significant loss in energy resolution is seen when summing all pixels even after more than one day of continuous counting. The spectral response of the XRS has been photometrically calibrated between 300 eV and 10 keV [16] and was monitored on EBIT-I by recording the signal from an x-ray tube attached to the opposite viewport.

The XRS's ∼10 eV resolution across the 700–1500 eV band is sufficient to resolve the strongest Fe XVII lines from one another, as shown in Fig. 1. We fielded a set of high-resolution crystal spectrometers [17] to detect blending with Fe XVI. A significant amount of Fe^{15+} is present only during the injection phase of the cycle when the iron ions are coming to equilibrium. These data were excluded from analysis by taking advantage of the ability to measure time-resolved spectra with both the crystal spectrometer and the XRS, and any remaining influence of Fe XVI line emission on the Fe XVII lines is determined as a small correction.

The radiative recombination (RR) emission from the capture of a beam electron by Fe^{16+}

ions can be seen in Fig. 1. It is described by:

$$
\begin{aligned}
1s^2 2s^2 2p^6 + e^- &\rightarrow 1s^2 2s^2 2p^6 3s_{1/2} + h\nu_1, \\
1s^2 2s^2 2p^6 + e^- &\rightarrow 1s^2 2s^2 2p^6 3p_{1/2} + h\nu_2, \\
1s^2 2s^2 2p^6 + e^- &\rightarrow 1s^2 2s^2 2p^6 3p_{3/2} + h\nu_3, \\
1s^2 2s^2 2p^6 + e^- &\rightarrow 1s^2 2s^2 2p^6 3d_{3/2} + h\nu_4, \\
1s^2 2s^2 2p^6 + e^- &\rightarrow 1s^2 2s^2 2p^6 3d_{5/2} + h\nu_5
\end{aligned} \tag{1}
$$

The energy difference between states of different orbital angular momentum, ℓ, is on the order of 40–50 eV and are resolved. However, the difference between states with the same ℓ is ≤ 2 eV and are not resolved predominantly because of the energy spread in the electron beam. The electron beam energy of the measurement is 964 ± 5 eV with a full width at half maximum of ~ 20 eV, as determined from fitting the RR peaks. This energy is consistent with the applied potential. The electron beam current for these measurements is 25 mA, giving an electron density of $10^{-10} \leq n_e \leq 10^{-11} cm^{-3}$. Note that the there are $\sim 10^5$ total counts in the line 3C in Figure 1, which is needed to accumulate more than 100 counts in the weakest radiative capture peak.

Utilizing the techniques developed in [12, 13] we normalize the measured intensities of lines $3C$ and $3D$ to the measured intensity of the RR peak, and in turn to the cross section for electron capture. The cross sections for RR are determined from the theory given by [18], which has been deemed accurate to within 5 % or better provided the electron energy is high, as it is in our case (see Table I). Polarization must be accounted for because of the mono-directional electron beam and the 90° viewing angle. The values of the polarization of the emitted radiation of $P = 1$ for $3s$ capture, 0.82 for $3p$, and 0.57 for $3d$ capture are provided by the same theory as the RR cross sections. The polarizations for direct excitation are calculated using the theory of [19] and are $P = 0.40$ for both $3C$ and $3D$.

The excitation cross sections inferred for $3C$ based on normalizing to each of the three observed RR peaks are given in Table I. The error associated with each measurement includes contributions from counting statistics, quantum efficiency, filter transmission, background subtraction, and polarization. We note that no Fe^{17+} exists at this beam energy. Hence, no enhancement of the Fe^{17+} lines resulting from recombination onto Fe XVIII is possible. Similarly, innershell ionization of Fe XVI cannot contribute.

If present, background ions with ionization energies near that of Fe^{16+} can contribute to the Fe XVII RR spectrum. For example, recombination onto C^{5+} or Fe^{15+} produces photons that will fall into a same energy range as recombination onto the Fe^{16+} $3d$ levels. Recombination onto Ar^{8+} and Ar^{9+} will fall into a similar energy range. We noticed a small enhancement at photon energies of ~ 1355 eV and 1395 eV, that we tentatively identify as RR onto C^{5+} and Ar^{8+}. However, the agreement between the three cross sections derived by normalizing separately to the three diffferent RR peaks shows the internal consistency of the measurement, intimating that no significant contribution from background ions exists. The average cross section of $3C$ is given in Table II.

Before deriving the cross section for the intercombination line $3D$, we took into account potential contributions from the Fe^{15+} inner-shell satellites, as indicated by the crystal spectrum, using the procedure discussed in [7]. After correcting for the Fe XVI contribution we obtained an intensity ratio of $I_{3D}/I_{3C} = 2.98 \pm 0.3$, in excellent agreement with previous measurements and tabulated theoretical ratios given in [11].

Table II summarizes the measured cross sections and compares them with the R-matrix calculations of Mohan et al. [20], the fully relativistic distorted-wave calculations of Zhang & Sampson [21], and the recent closed-coupling (R-matrix) calculations of Chen & Pradhan [11]. All these calculations include configuration interaction and cascade contributions from levels up to $n = 4$. However, only Chen & Pradhan [11] include resonance excitation. We use their 30 eV Gaussian-averaged collision strengths to derive the cross sections listed.

Table II shows that our measured cross section of $3D$ agrees with the DW value and the resonance free R-matrix calculation. It is 30 % lower than the result of the 89 level CC calculation given by Chen & Pradhan. The measured cross section for $3C$ does not agree with any of the three theories. It is 35 % lower than the value of Zhang & Sampson, 26 % lower than Mohan et al., and 50 % lower than that of Chen & Pradhan, as is illustrated in Fig. 2. Clearly, the two calculations that do not include resonances agree better with our measured values than the values of Chen & Pradhan.

We also measured the excitation cross sections as a function of electron-impact energy utilizing an event-mode method in which the electron beam is swept linearly between two energies and each photon is tagged with the corresponding electron beam energy [22]. The results are plotted in Fig. 3. The results of the R-matrix calculations with and without resonances are shown for comparison. The resonance-free R-Matrix calculation is in excellent agreement for line $3D$. Within the resolution and accuracy of the experiment no strong enhancement from resonances are detected in 3D. For line $3C$ the resonance free calculations correctly predict the measured shape of the energy dependence, but, as noted above, the values are too large by a factor of 1.4. The addition of resonances only adds further to the discrepancy. Again, there is no obvious signature in the experimental data of the effect of resonances on the excitation cross section of line $3C$. From our results we conclude that resonances only play a minor role in the excitation of the upper level of 3C and 3D as previously stated in [23]. In addition, although Chen & Pradhan do not include resonances from $n \geq 5$, their inclusion would increase the discrepancy between experiment between theory and experiment. Our finding that resonances do not play a large role in enhancing $3C$ and $3D$ in neonlike Fe XVII agrees with an earlier study of indirect line excitation processes in high-Z neon-like ions and supports the modeling approach recently given by Fournier & Hansen [24] where disagreement from experiment was reduced from ~ 20 % to ~ 10 % without the inclusion of resonances.

In summary, we have established a new benchmark for calculating cross sections of medium-Z neonlike ions. The new results for the first time go beyond relative line ratios and they establish the possibility of using microcalorimeters for measuring cross sections of soft X-ray transitions in low and medium-Z ions inaccessible by earlier techniques. Resonance enhancement is found to be weak. Our measurement has important implications for the analysis of astrophysical spectra and eliminates the need for invoking resonance scattering for explaining the reduced emission of 3C observed in many astrophysical sources relative to that expected from calculations. Correct abundance measurements can be obtained by using the cross sections resulting, for example, from distorted-wave calculations for $3D$ but not for $3C$. Our measurements thus resolves the puzzling observations by Xu et al. [3] and Behar et al. [2] who in their study of NGC 4656 and Capella, respectively, found that consistent results were obtained only if they normalized their *Chandra* spectrum to $3D$ not to $3C$. The surprising weakness of the cross section of the dominant Fe XVII line also removes the remaining discrepancy between model calculations based on distorted-wave cross sections and observations of the intensity of the $3s \rightarrow 2p$ lines relative to those of line $3C$ discussed in [9].

We acknowledge E. Magee, P. D'Antonio, and J. Gygax for their technical support, and M. F. Gu for stimulating discussions. Work by the Univ. of California Lawrence

Livermore Nat'l Laboratory was performed under the auspices of the D.o.E. under contract No. W-7405-Eng-48 and supported by NASA APRA grants to LLNL, GSFC, and Stanford University.

[1] C. R. Canizares, D. P. Huenemoerder, D. S. Davis, K. A. Flanagan, J. Houck, T. H. Markert, H. L. Marshall, M. L. Schattenburg, N. S. Schulz, M. Wise, et al., Astrophys. J. Lett. **539**, L41 (2000); A. C. Brinkman, E. Behar, M. Gudel, A. J. F. den Boggende, G. Braunduardi-Raymont, J. Cottam, C. Erd, J. W. den Herder, F. Jansen, J. S. Kaastra, et al., Astron. Astrophys. **365**, L324 (2001); S. M. Kahn, M. A. Leutenegger, J. Cottam, G. Raun, J. M. Vreux, A. J. F. den Boggende, R. Mewe, and M. Güdel, Astron. Astrophys. **365**, L312 (2001).

[2] E. Behar, J. Cottam, and S. M. Kahn, Astrophys. J. **548**, 966 (2001).

[3] H. Xu, S. M. Kahn, J. R. Peterson, E. Behar, F. B. S. Paerls, R. F. Mushotzky, J. G. Jernigan, and K. Makishima, Astrophys. J. **579**, 600 (2002).

[4] D. L. McKenzie, P. B. Landecker, R. M. Broussard, H. R. Rugge, and R. M. Young, Astrophys. J. **241**, 409 (1980); K. J. H. Phillips, C. J. Greer, A. K. Bhatia, I. H. Coffey, R. Barnsley, and F. P. Keenan, Astron. Astrophys. **324**, 381 (1997).

[5] J. H. Parkinson, Astron. Astrophys. **24**, 215 (1973); K. Waljeski, D. Moses, K. Dere, J. L. R. Saba, D. F. Web, and D. M. Zarro, Astrophys. J. **429**, 909 (1994).

[6] K. Wood and J. Raymond, Astrophys. J. **540**, 563 (2000).

[7] G. V. Brown, P. Beiersdorfer, H. Chen, M. H. Chen, and K. J. Reed, Astrophys. J. Lett. **557**, L75 (2001).

[8] G. V. Brown, P. Beiersdorfer, S. M. Kahn, D. A. Liedahl, and K. Widmann, Astrophys. J. **502**, 1015 (1998); P. Beiersdorfer, M. Bitter, and S. von Goeler, Astrophys. J. **610**, 616 (2004).

[9] P. Beiersdorfer, E. Behar, K. R. Boyce, G. V. Brown, H. Chen, K. C. Gendreau, M.-F. Gu, J. Gygax, S. M. Kahn, R. L. Kelley, et al., Astrophys. J. Lett. **576**, L169 (2002).

[10] P. Beiersdorfer, S. von Goeler, M. Bitter, and D. B. Thorn, Phys. Rev. A **64**, 032705 (2001).

[11] G. X. Chen and A. K. Pradhan, Phys. Rev. Lett. **89**, 013202 (2002).

[12] R. E. Marrs, M. A. Levine, D. A. Knapp, and J. R. Henderson, Phys. Rev. Lett. **60**, 1715 (1988).

[13] K. L. Wong, P. Beiersdorfer, K. J. Reed, and D. A. Vogel, Phys. Rev. A **51**, 1214 (1995).

[14] C. K. Stahle, D. McCammon, and K. D. Irwin, Phys. Today **47**, 27 (1999).

[15] R. L. Kelley, M. D. Audley, K. R. Boyce, S. R. Breon, R. Fujimoto, K. C. Gendreau, S. S. Holt, Y. Ishisaki, D. McCammon, T. Mihara, et al., SPIE **3765**, 114 (1999); F. S. Porter, M. D. Audley, P. Beiersdorfer, K. R. Boyce, R. P. Brekosky, G. V. Brown, K. C. Gendreau, J. Gygax, S. M. Kahn, R. L. Kelley, et al., in *Proceedings of the 45th annual SPIE meeting on Optical Science and Technology* (SPIE Press, 2000), p. 4140.

[16] M. D. Audley, R. Fujimoto, K. Mitsuda, K. Arnaud, K. C. Gendreau, K. R. Boyce, C. M. Fleetwood, R. L. Kelley, R. A. Keski-Kuhn, F. S. Porter, et al., in *Proceedings of a New Century of X-ray Astronomy*, Astronimical Society of the Pacific (Astronimical Society of the Pacific, San Francisco, CA, 2001), p. 516.

[17] G. V. Brown, P. Beiersdorfer, and K. Widmann, Rev. Sci. Instrum. **70**, 280 (1999).

[18] E. Saloman, J. Hubell, and J. Scofield, At. Data Nucl. Data Tables **38**, 1 (1988).

[19] H. L. Zhang, D. H. Sampson, and R. E. H. Clark, Phys. Rev. A **41**, 198 (1990).

[20] M. Mohan, R. Sharma, and W. Eissner, Astrophys. J. **108**, 389 (1997).

[21] H. L. Zhang and D. H. Sampson, At. Data Nucl. Data Tables **43**, 1 (1989).

[22] D. Knapp, Z. Phys. D **S21**, S143 (1991); P. Beiersdorfer, G. V. Brown, L. . Hildebrandt, K. L. Wong, and R. Ali, Rev. Sci. Instrum. **72**, 508 (2001).

[23] W. H. Goldstein, A. L. Osterheld, J. Oreg, and A. Bar-Shalom, Astrophys. J. Lett. **334**, L37 (1989); P. Beiersdorfer, A. L. Osterheld, M. H. Chen, J. R. Henderson, D. A. Knapp, M. A. Levine, R. E. Marrs, K. J. Reed, M. B. Schneider, and D. A. Vogel, Phys. Rev. Lett. **65**, 1995 (1990); M. F. Gu, Astrophys. J. **582**, 1241 (2003); R. Doron, and E. Behar, Astrophys. J. **574**, 2002 (1990). .

[24] K. B. Fournier, and S. B. Hansen, Phys. Rev. A (in press).

TABLE I: Results of the measurements at an electron impact energy of 964 eV of the resonance line 3C normalized to each of the different RR states.

RR states used for normalization	$\sigma_{RR}(cm^2)$ at 90°	$\sigma_{3C}(cm^2)$
$3s_{1/2}$	5.34×10^{-23}	$8.93 \pm 1.6 \times 10^{-20}$
$3p_{1/2} + 3p_{3/2}$	1.23×10^{-22}	$8.81 \pm 1.5 \times 10^{-20}$
$3d_{3/2} + 3d_{5/2}$	3.90×10^{-23}	$8.92 \pm 1.7 \times 10^{-20}$

TABLE II: Comparison of measured and calculated cross sections for the Fe XVII resonance and intercombination x-ray lines.

Line	E_{e^-} (eV)	σ $(cm^2)^a$	Theory ^{b}	Theory^c	Theory^d
3C	964	$8.88 \pm 0.93 \times 10^{-20}$	1.12×10^{-19}	1.19×10^{-19}	1.33×10^{-19}
3D	964	$2.98 \pm 0.33 \times 10^{-20}$	2.83×10^{-20}	3.14×10^{-20}	3.93×10^{-20}

[a]This measurement

[b]Mohan et al. 1997 [20]. These cross sections are calculated for 1088 eV.

[c]Zhang & Sampson 1989 [21]

[d]Chen & Pradhan 2002 [11]. These values are estimated from the collision strengths given in their figure1(a) for 3C and 1(b) for 3D.

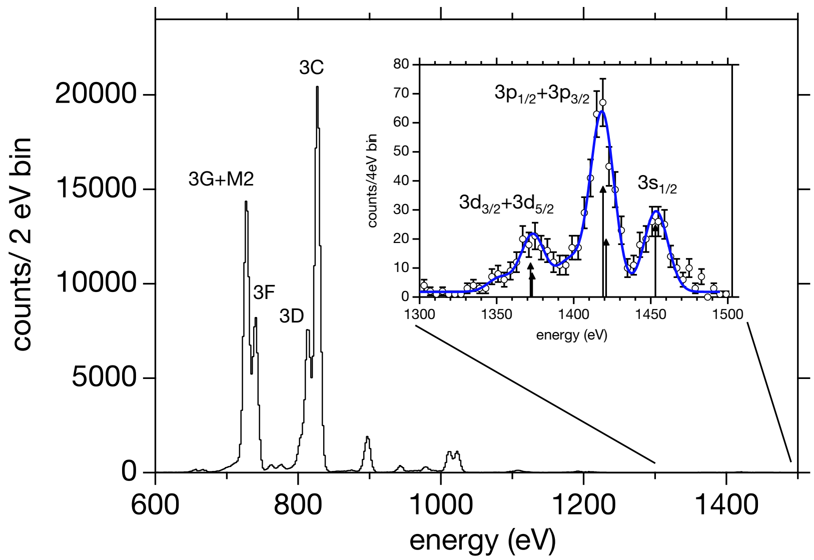

FIG. 1: Spectrum of Fe XVII measured by the NASA/GSFC 6 $\times$ 6 microcalorimeter array. The insert shows a close up view of the energy range containing the photons from radiative recombination. The peaks are labelled with the different fine structure components of Fe XVI. This spectrum is not corrected for filter transmittance or polarization effects.

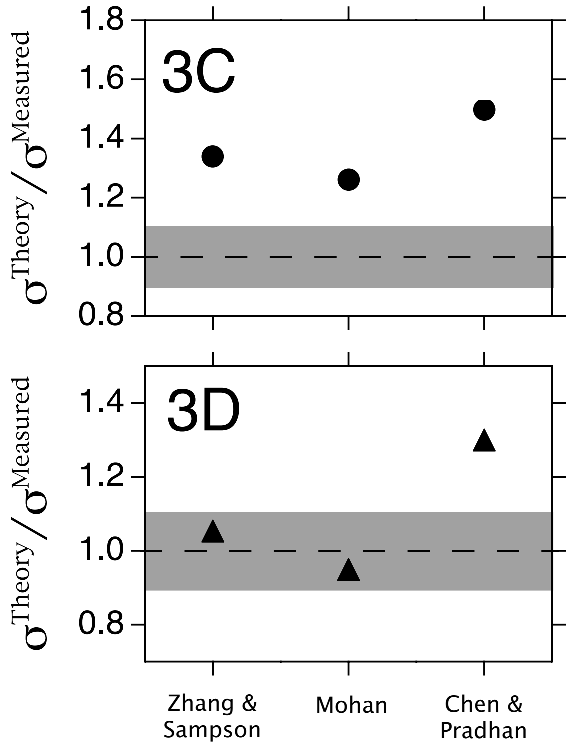

FIG. 2: Theoretical cross sections normalized to measured cross for the resonance line 3C and the intercombination line 3D. The error on the measured values is indicated here by the gray area in each plot.

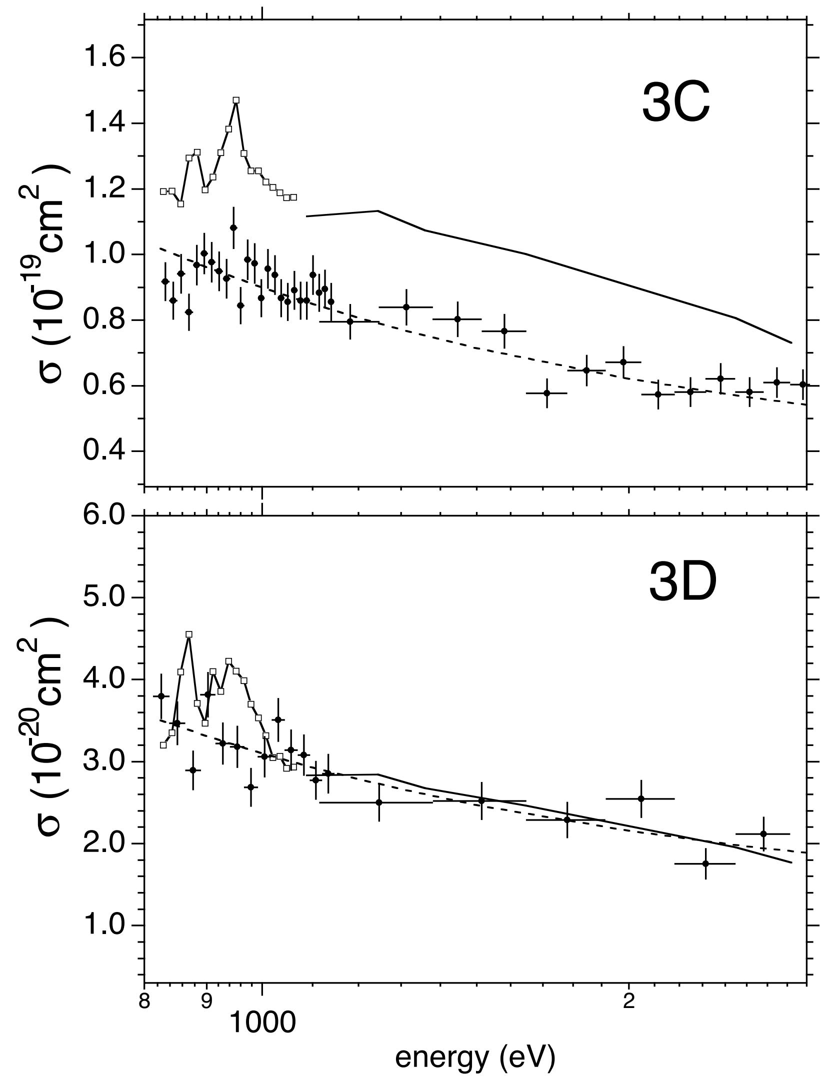

FIG. 3: Cross sections for the resonance line 3C (top) and intercombination line 3D (bottom) as a function of electron-impact energy given by closed circles. The error bars in the y direction are statistical and the error bars in the x direction denote the bin size. These points are normalized to the single-energy measurement at E_{e-}= 964 eV. The dashed line in each plot is a power law fit to the experimental data with $\sigma \propto E^{-1}$. Each cross section is compared to the theories of Mohan et al. 1997 [20] (solid line) and Chen & Pradhan [11] (open squares on solid line).